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The Terascale Simulation Tools and Technologies Center

David Brown *(Lawrence Livermore)*

Lori Freitag *(Argonne)*

Jim Glimm *(Brookhaven, SUNY Stony Brook)*

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http://www.tstt-scidac.org/

Terascale
Simulation
Tools
and
Technologies

TSTT

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The TSTT Center

- *Goal:* To enable high-fidelity calculations based on multiple coupled physical processes and multiple physical scales
  - *Adaptive methods*
  - *Composite or hybrid solution strategies*
  - *High-order discretization strategies*

- *Barrier:* The lack of easy-to-use interoperable meshing, discretization, and adaptive tools requires too much software expertise by application scientists

The TSTT center recognizes this gap and will address the technical and human barriers preventing use of adaptive, composite, hybrid methods

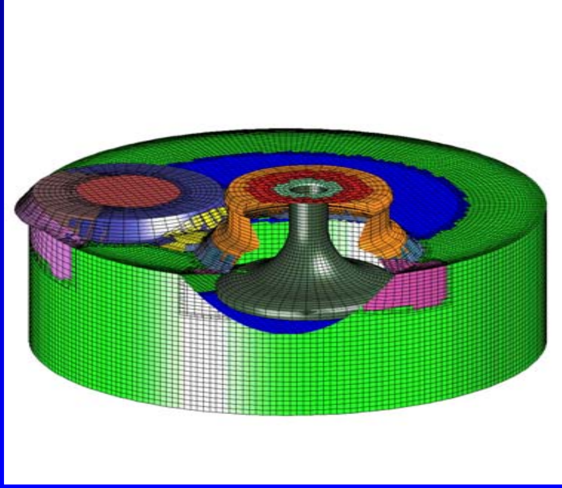
TSTT Participants

- ANL: Fischer, *Freitag*, Leurent, Tufo
- BNL: *Glimm*, Samulyak
- LLNL: *Brown*, Chand, Fast, Henshaw, Quinlan
- ORNL: *D' Azevedo*, de Almeida, Khamayseh
- PNNL: *Trease*
- RPI: Flaherty, Hau, Remacle, *Shephard*
- SNL: Brewer, *Knupp*, Melander, Tautges
- SUNY SB: Glimm, *Li*

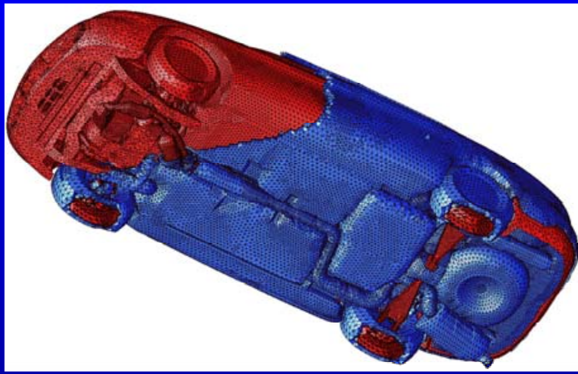
**Italics denote site PI*

TSTT brings together meshing and discretization expertise from DOE Labs and Universities

- **Structured meshes**
  - **Overture** - high quality, predominantly structured meshes on complex CAD geometries (LLNL)
  - Variational and Elliptic Grid Generators (ORNL, SNL)
- **Unstructured meshes**
  - **AOMD** (RPI) - primarily tetrahedral meshes, boundary layer mesh generation, curved elements, AMR
  - **CUBIT** (SNL) - primarily hexahedral meshes, automatic decomposition tools, common geometry module
  - **NWGrid** (PNNL) - hybrid meshes using combined Delaunay, AMR and block structured algorithms
  - **Frontier** (BNL) – interface front tracking



Overture Mesh (LLNL)



MEGA Boundary Layer Mesh (RPI)

Bringing this sophisticated technology to DOE application scientists is the challenge

- These tools all meet particular needs, but
  - They do not interoperate to form hybrid, composite meshes
  - They cannot be easily interchanged in an application
- In general the technology requires too much software expertise from application scientists
  - Difficult to improve existing codes
  - Difficult to design and implement new codes

We meet this challenge through a 2-pronged approach

Near term collaborations helps us understand application requirements …

- *Near term:* deployment of current TSTT mesh and discretization capabilities by partnering with SciDAC applications
- *Long term:* development of interoperable software tools enabling
  - Rapid prototyping of new applications
  - Plug-and-play insertion of mesh and discretization technology through uniform software interfaces

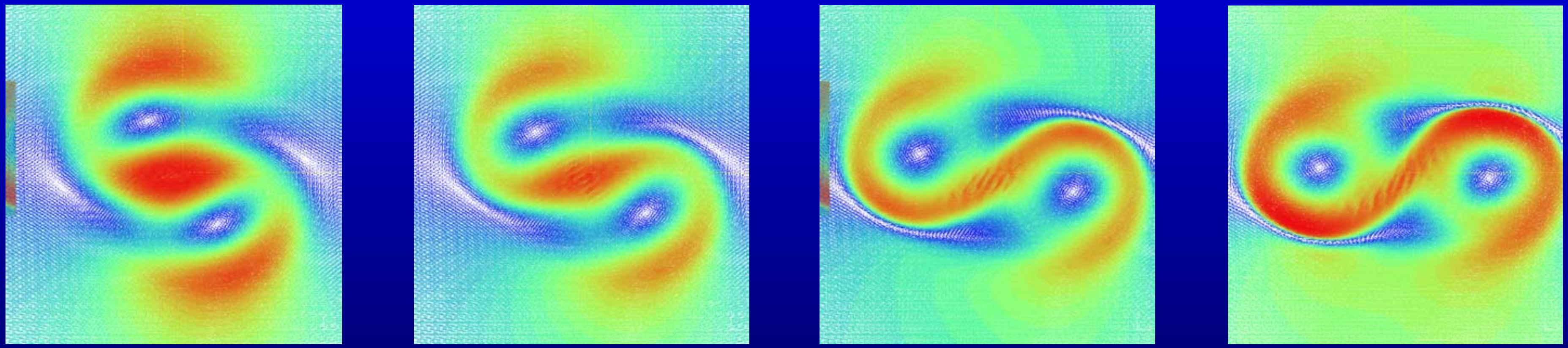
… feeding into interface design of future software components

Near Term Strategy

- Interact with SciDAC Applications to develop working relationships in each application area by
  - Analyzing the needs of application scientists
  - Inserting existing TSTT technology
    - Provides a short-term impact for application scientists
    - Builds trust relationship
  - Developing new technologies for later insertion and new application development
- Key application areas: Fusion, Astrophysics, Accelerator Design, Climate

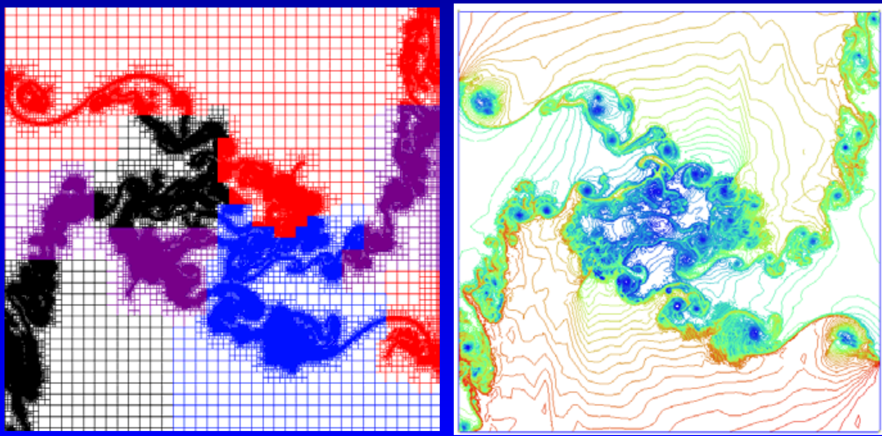
High-Order FEM for Fusion

- High-order, adaptive finite element techniques for magneto-hydrodynamics
  - Fusion PI: Jardin/Strauss (PPPL)
  - TSTT PI: Shephard/Flaherty (RPI)
  - *Goal:* To test high-order and adaptive techniques; compare to existing linear FEM
  - *Progress:*
    - Initial results obtained for both potential and primitive variable mixed formulations for the 2D adipole vortex flow pattern
      - Two oppositely directed currents embedded in a constant magnetic field which holds them in an unstable equilibrium
      - They compress and rotate to align with magnetic field to reduce energy (see below)
    - Beginning to test high-order and h-adaptive techniques available in Trellis to determine applicability to this problem
    - Quadratic and cubic results presented by J.E. Flaherty earlier today



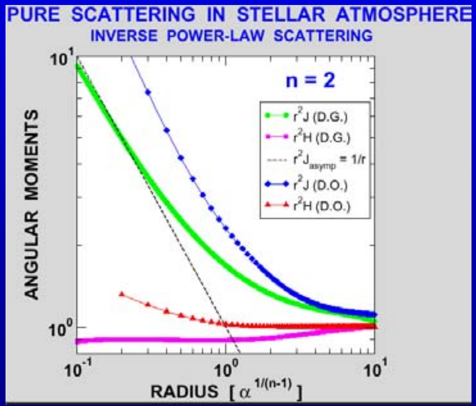
Adaptive DG for Astrophysics

- Contact instabilities in hydrodynamics
  - Application PI: Bhattacharjee/Rosner (Iowa/UofC)
  - TSTT PI: Shephard (RPI)
  - *Goal:* to test h-p adaptive DG in hydrodynamics; compare to existing PPM
  - *Progress:* 3-D adaptive test to 256 processors have been done in Trellis for four contact Riemann problem



Adaptive mesh and density contours after structures have evolved. Colors on right mesh indicates processor assignment for this 4 processor case

- Boltzman transport equations for neutrinos
  - Application PI: Mezzacappa (ORNL)
  - TSTT PI: de Almeida (ORNL)
  - *Goal:* to eliminate barriers imposed by discrete ordinates discretization (non-adaptive, compuationally intensive) by developing a discontinuous Galerkin alternative
  - *Progress:* adaptive DG shows strong exponential decay, energy conservation, and outward peaking and gives better results than Discrete Ordinates

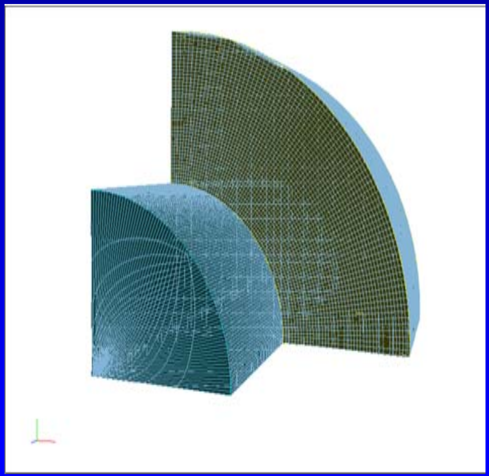


DOM does not reach asymptotic limit at large optical depth and does not conserve energy

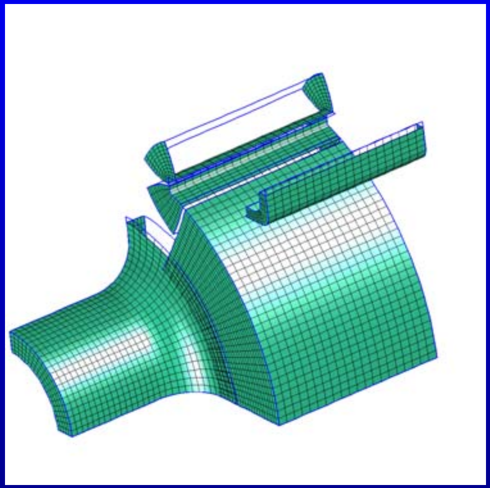
Adaptivity in DGM provides more accuracy the slight loss of energy will be corrected

Mean Radiation Intensity (J); Net Energy Flux (H)

Mesh Quality in Accelerator Design

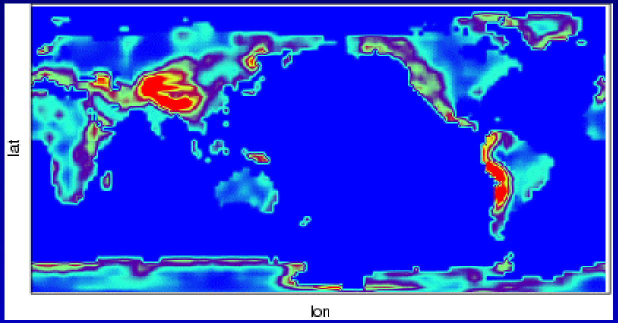


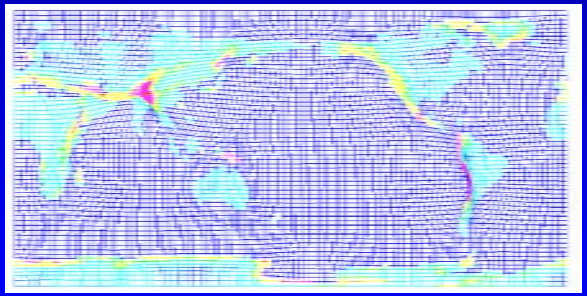
- Understanding the effect of mesh quality on Tau3P
  - Application PI: Ko/Folwell (SLAC)
  - TSTT PI: Knupp (SNL), Henshaw (LLNL)
  - *Goal:* Determine the mesh quality factors that most affect stability of Tau3P and to devise discretization schemes to improve the stability of Tau3P without affecting long-time accuracy
  - *Progress:*
    - Systematic mesh quality analysis using CUBIT meshes revealed that run time varies by a factor of 3 from “best” to “worst” mesh and that smoothness and orthogonality are the most important factors
    - Analytically derived sufficient conditions on mesh quality for stability of discretization in Tau3P
    - Implemented basic Tau3P discretization strategy in Overture and analyzing feasibility of schemes stabilizing the DSI method

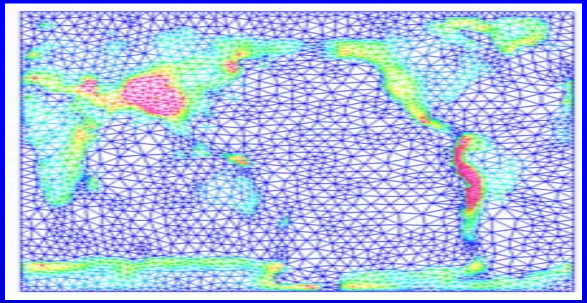


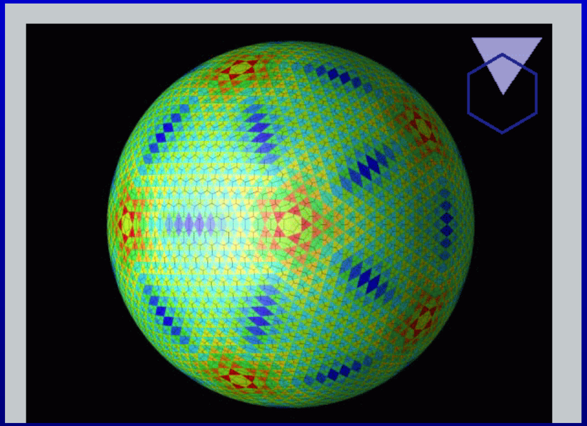
Climate

- Adaptive gridding to minimize solution error
  - Application PI: Drake (ORNL)
  - TSTT PI: Khamayseh (ORNL)
  - *Goal:* Given an initial isotropic or anisotropic planar or surface mesh and a solution field with large gradient mountain heights, use solution based r-adaptation to minimize solution error
  - *Progress*: Proof of principle of meshing technologies demonstrated
- Geodesic mesh quality improvement
  - Application PI: Randall/Ringler (Colorado)
  - TSTT PI: Knupp (SNL)
  - *Goal:* Create smoothed geodesic grids to improve calculation accuracy
    - Plan to use early version of Mesquite to create smoothed grids with respect to element area and perform calculations with smoothed grids to determine effect in Fall '02



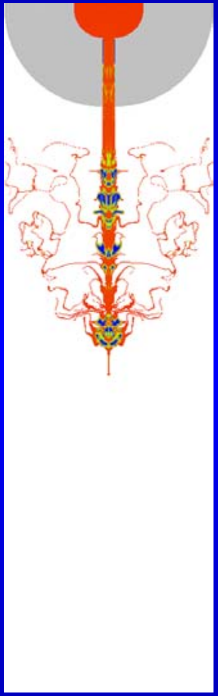


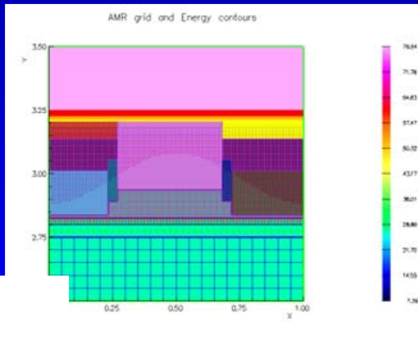


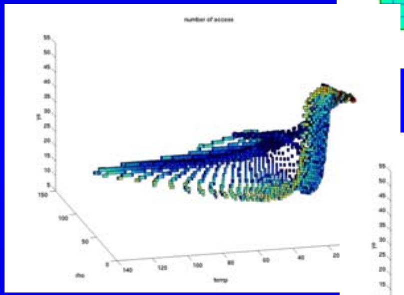


Other examples where TSTT technology is helping near-term application progress

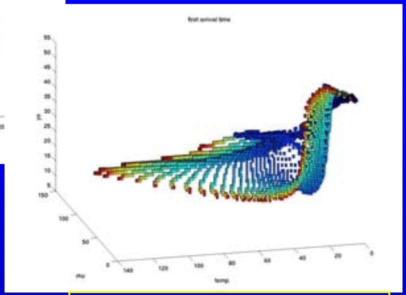
- Front tracking and adaptive techniques in Frontier and Overture for modeling of the breakup of a diesel fuel jet into spray (Argonne/BNL)
- 3D caching schemes to avoid redundant, costly evaluations of scattering kernels in phase space in astrophysics calculations (ORNL/ORNL)
- Mesh-based schemes for computational biology applications such as rat olfactory systems and human lungs (PNNL/PNNL)
- Low-order FEM schemes used as effective preconditioners in Climate applications (Colorado/ANL)



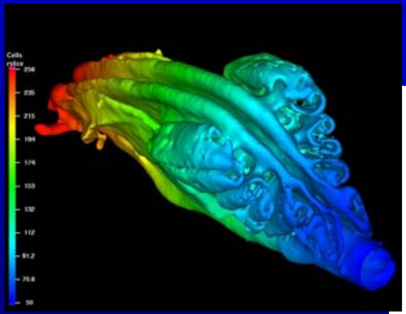


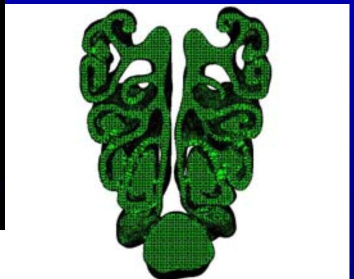


Access pattern :red is more frequent



Access sequence: red is accessed late in simulation





Long Term Strategy

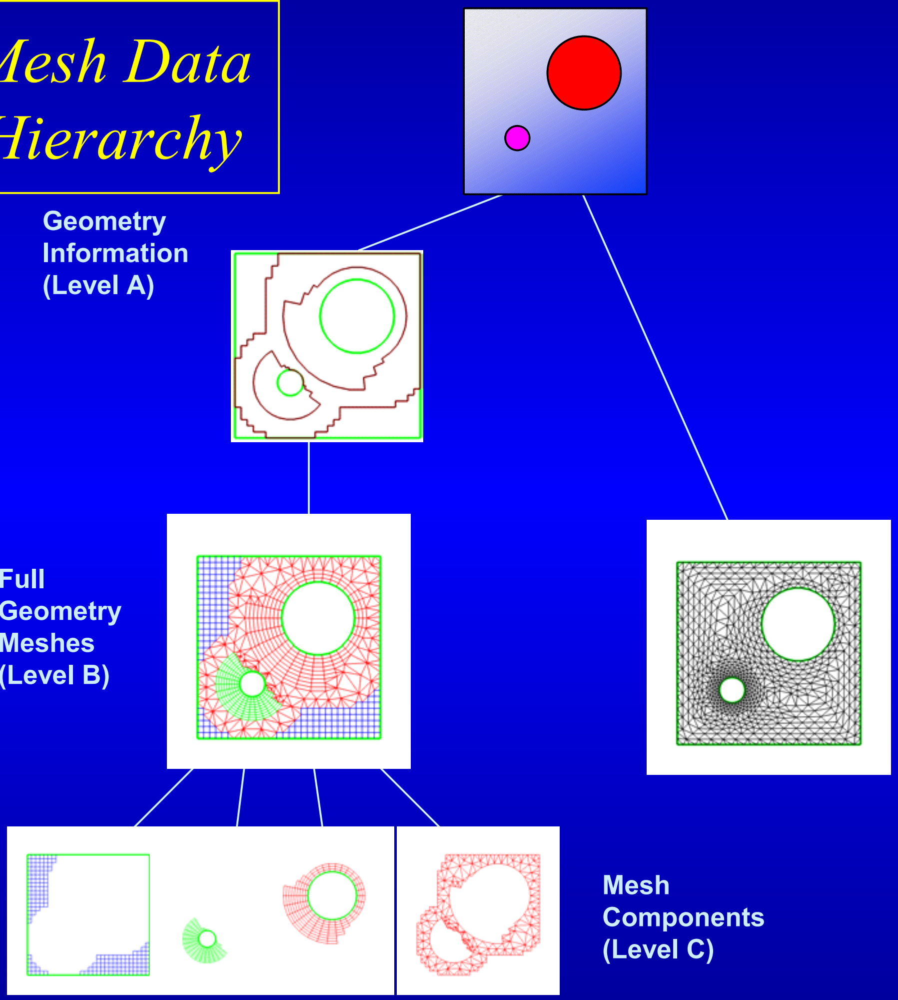
- Create interoperable meshing and discretization components
  - Common interfaces for mesh query and modification
  - Initial design will account for interoperability at all levels
  - Encapsulate existing TSTT software tools into CCA-compliant components for plug and play

- Develop new technologies as needed to enable interoperability
  - High-level discretization library
  - Mesh quality improvement for hybrid meshes
  - Terascale algorithms for adaptivity, load balancing, interpolation

Access to geometrical information is provided at different levels of abstraction

- **Level A: Geometric description of the domain**
  - provides a common frame of reference for all tools
  - facilitates multilevel solvers
  - facilitates transfer of information in discretizations
- **Level B: Full geometry hybrid meshes**
  - mesh components
  - communication mechanisms that link them (key new research area)
  - allows structured and unstructured meshes to be combined in a single computation
- **Level C: Mesh Components**

Mesh Data Hierarchy



Access through both low and high level interfaces

Low Level Access

- Access the mesh through the individual components
- For example
    - element-by-element access to mesh components
    - fortran-callable routines that return interpolation coefficients at a single point (or array of points)
- Facilitates incorporation into existing applications

Mesh Component Interface Specification

- **Philosophy**
  - Create a small set of interfaces that existing packages can support
  - Balance performance and flexibility
  - Work with a large tool provider and application community to ensure applicability
- **Status**
  - Nomenclature is determined
  - Interfaces for basic access to mesh geometry and topology
  - Prototype implementations
    - All TSTT sites
    - C, C++, and Fortran
- **To Do**
  - Parallel query, mesh services, canonical orderings, mesh modification, structured mesh interfaces,tags…
  - Interaction with discretization strategies and DOF managers

Issues that have arisen

- Nomenclature is harder than we first thought
- Cannot achieve the 100 percent solution, so...
  - What level of functionality should be supported?
    - Minimal interfaces only?
    - Interfaces for convenience and performance?
  - What about support of existing packages?
    - Are there atomic operations that all support?
    - What additional functionalities from existing packages should be required?
  - What about additional functionalities such as locking?
- Language interoperability is a problem
  - Most TSTT tools are in C++, most target applications are in Fortran
  - How can we avoid the “least common denominator” solution?
  - Exploring the SIDL/Babel language interoperability tool

Mitigating the Risks

- *Risk:* The technology won't be adopted by application scientists or tool developers

  Mitigated by

  - Providing new capabilities to applications that are needed but not otherwise accessible
  - Building relationships with application scientists now
    - Builds trust
    - Demonstrates desirability of the technology
  - Keeping the interfaces simple, minimal, adoptable
- *Risk:* We shoot too high and deliver nothing

  Mitigated by

  - Understanding that this is a risk and accepting the 80% solution when necessary
  - Delivering interface capabilities incrementally (e.g., first query, then modification)

High Level Access

- Operate on the mesh components as though they were a single mesh object
  - Discretization operators
  - Mesh modifications
    - Mesh quality improvement
    - Refinement/coarsening
  - Error estimation
  - Multilevel data transfer
- Prototypes provided by Overture and Trellis frameworks
- Enables rapid development of new mesh-based applications

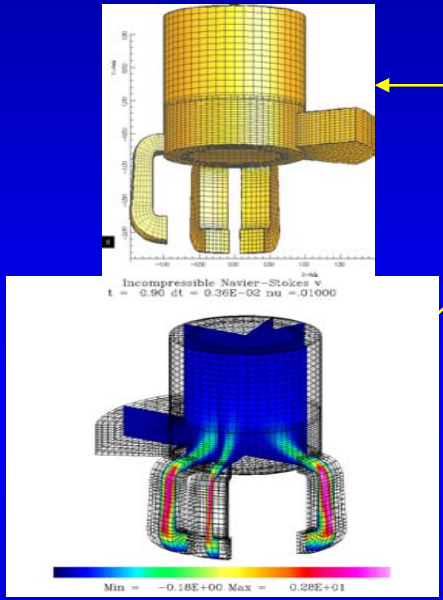
Discretization Library

- *Observation:* Complexities of using high-order methods on adaptively evolving grids has hampered their widespread use
  - Tedious low level dependence on grid infrastructure
  - A source of subtle bugs during development
  - Bottleneck to interoperability of applications with different discretization strategies
  - Difficult to implement in general way while maintaining optimal performance
- Result has been a use of sub-optimal strategies or lengthy implementation periods
- *TSTT Goal:* to eliminate these barriers by developing a *Discretization Library*

Functionalities

- Mathematical operators will be implemented
  - Start with +, -, *, /, interpolation, prologation
  - Move to div, grad, curl, etc.
  - Both strong and weak (variational) forms of operators when applicable
- Many discretization strategies will be available
  - Finite Difference, Finite Volume, Finite Element, Discontinuous Galerkin, Spectral Element, Partition of Unity
  - Emphasize high-order and variable-order methods
  - Extensive library of boundary condition operators
- The interface will be independent of the underlying mesh
  - Utilizes the common low-level mesh interfaces
  - All TSTT mesh tools will be available
- Interface will be extensible, allowing user-defined operators and boundary conditions

Example provided by Overture prototype



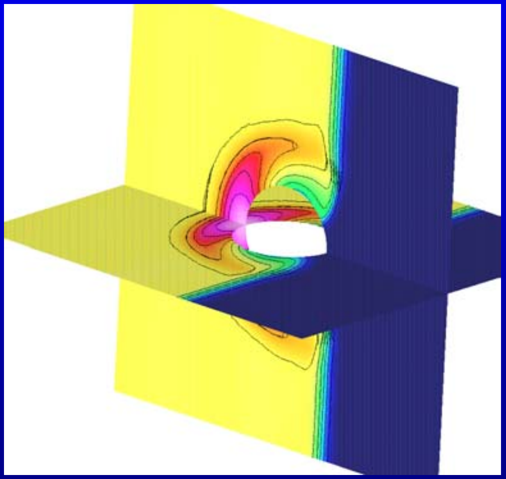

```
CompositeGrid cg;
floatCompositeGridFunction u,v,w;

v = u.y();
w = u.laplacian();

Plotstuff ps;
ps.plot (cg);
ps.contour (w);
```

Differentiation Operators

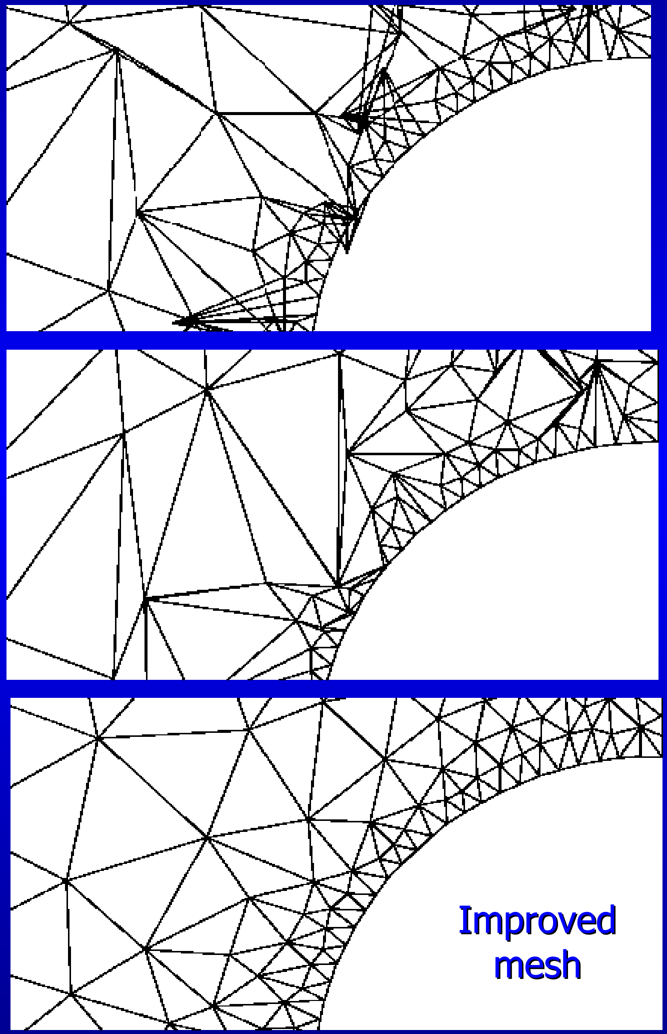
Visualize grid and data



Trellis (RPI) provides similar capability for finite-element method

MESQUITE Mesh Quality Improvement

- *Goal*: To provide a stand-alone tool for mesh quality improvement
  - hybrid, component based meshes
  - development of quality metrics for high order methods
  - a posteriori quality control using error estimators
- *Methods*
  - optimization-based smoothing and untangling (based on Opt-MS and CUBIT algorithms)
  - reconnection schemes
- *Status*
  - Prototype designed and most classes implemented for a simple optimization algorithm
  - Opt-MS and CUBIT algorithms inserted this summer
  - Built on TSTT interface
- *SciDAC Application Impact*
  - SLAC mesh quality improvement
  - Geodesic grids in climate
  - Integrated with CUBIT, NWgrid, Overture, AOMD



SciDAC ISIC Collaborations

- TOPS: (PI: Keyes)
  - provide mesh representations for multilevel techniques
  - co-develop well-defined interfaces to ensure that the meshes and discretization strategies will be interoperable with solution software
- APDEC: (PI: Colella)
  - provide mesh generation technologies via Overture
  - co-develop common interfaces for block structured AMR strategies
- CCA: (PI: Armstrong)
  - co-develop common interfaces for mesh and field data
  - create CCA-compliant mesh components and provide them in the CCA component repository
  - explore the role of the component model in the composition of numerous discrete operators
- Performance: (PI: Bailey)
  - we will use *ROSE* preprocessor to develop highly-tuned discretization libraries
  - TSTT will provide benchmarks and a testing environment for developments in the performance ISIC

Summary

The TSTT Center focuses on interoperable meshing and discretization strategies on complex geometries

- Short term impact through technology insertion into existing SciDAC applications
- Long term impact through the development of
  - a common mesh interface and interoperable and interchangeable mesh components
  - new technologies that facilitate the use of hybrid meshes
- Working with SciDAC ISICs to ensure applicability of tools and interfaces

Contact Information

- TSTT Web Site: www.tstt-scidac.org

- David Brown: dlb@llnl.gov
- Lori Freitag: freitag@mcs.anl.gov
- Jim Glimm: glimm@ams.sunysb.edu

The End